# Location of Shoulders in Channeling Phenomena*

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A Monte Carlo computer program for use in calculating channeling effects has been written. It incorporates a model of lattice vibrations in which the lattice atoms vibrate independently of each other. The position of the shoulder for a planar channel is predicted quite well by the breakthrough angle for trajectories in the channel. The position of the shoulder of a row channel is found to be determined by the shoulders of the several planar channels intersecting at the row channel. The breakthrough angle for rows appears to mark a rather sharp boundary between orientations in which row or planar effects predominate.

CRITERIA for the validity of use in channeling calculations of continuum potentials for strings and planes of atoms have been discussed by Lindhard.[1] His criterion for breakthrough of a string potential has been compared by a number of experimenters[2–8] with their measured widths at half-minimum of the decrease in phenomena observed near major row directions. This article reports some calculations of channeling using a Monte Carlo computer program which lead to a different interpretation of the breakdown of a continuum potential. The location of the shoulder on a planar channel has been found to correspond to the orientation at which ions injected near the center of the channel have enough transverse kinetic energy to surmount the potential barrier of the planes bounding the channel. The location of the shoulder on a row channel has been found to be determined by the shoulders of planar channels passing through the row channel rather than by any simple feature of the rows themselves.

The present computer program has been written for calculating trajectories of high speed ions in a lattice and using these trajectories to predict nuclear reaction rates, emergent beam patterns, and other phenomena of interest. Random numbers are used to select a starting position for each trajectory and to approximate the effects of beam divergence, mosaic spread, and independent thermal vibrations of each lattice atom. The moving ions are assumed to have an important interaction with only one lattice atom at a time, and the impulse approximation is used to compute the deflection of the moving ion at each interaction. A variety of interaction potentials can be used in the calculations; mostly Molière's fit to the Thomas-Fermi function[9] with Firsov's screening length[10] has been used. At each interaction the probability of a nuclear reaction is computed. At the end of a series of trajectories, the accumulated probability is divided by the corresponding probability for a random direction. The resulting quotient is referred to as the nuclear reaction probability normalized to unity for a random direction.

Because of the extensive experimental work[3] on the orientation dependence of $(p,\gamma)$ reaction rates for 1.4-MeV protons in aluminum, calculations described herein have been done corresponding to these experimental conditions, with the temperature taken to be 40°C unless otherwise noted. Although the results to be presented show considerable agreement with these experiments, detailed comparison with experiment is not the purpose here. Rather, the author wishes to indicate the extent to which certain features of the results may be understood in a simple way from basic properties of the potential.

Figure 1 shows the results in the region of the shoulder of the $(1\bar{1}1)$ planar channel. The error bars shown on the points result from the Monte Carlo nature of the computations and indicate the standard deviation obtained from several calculations. From the figure it can be seen that both the height and location of the shoulder are dependent on depth and beam width. Although not shown here, the curves of Figs. 1(a) and 1(c) have been followed through the minimum at the center of the planar channel. The normalized reaction probabilities in the centers of the channels were calculated to be $0.43\pm0.05$ and $0.24\pm0.02$, respectively. The respective half-widths were found to be 0.17° and 0.18°. Because parts (a) and (b) of Fig. 1 are influenced by the effect of the surface, Fig. 1(c) corresponds more nearly to the response of the bulk of the crystal. The location of the peak in Fig. 1(c) should be given by the same rule that has been observed to apply for blocking[11]: The angle of the peak of the shoulder will be very nearly equal to the angle that gives trajectories entering the channel at its center just enough transverse kinetic energy to overcome the potential barrier of the planes. The breakthrough angle estimated in this way from the continuum planar potential averaged over thermal

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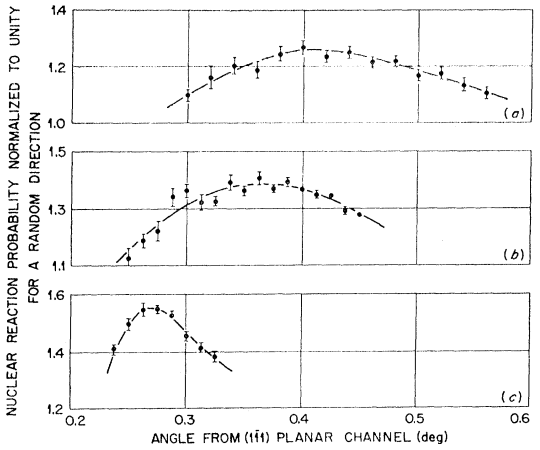


FIG. 1. Nuclear reaction probability across the shoulder of the (1$\bar{1}$1) planar channel at 5° from the [110] direction. The conditions for the graphs are as follows: (a) reaction range 0–286 Å (100 atoms) in from the surface, beam divergence 1.0°; (b) reaction range 0–286 Å, beam divergence 0°; (c) reaction range 0–1143° Å (400 atoms), beam divergence 0°.

vibrations[12] is 0.260°,[13] while the value obtained from Fig. 1(c) is 0.267°. For temperatures of 4 and 900°K, the breakthrough angles from the rule above are 0.275° and 0.240°, respectively, while the values from plots similar to Fig. 1(c) are found to be 0.275° and 0.255°, respectively. As seen from these results, the correspondence of the peak of the shoulder with the breakthrough angle is quite close for planar channeling in the absence of beam divergence and mosaic spread. The correspondence is less close when these two factors are present.

Some results obtained for nuclear reaction rates near the [110] row direction are shown in Fig. 2. For all three parts of this figure the beam divergence was 0.1° to correspond to experiment, and the depth was 100 atoms. The plane used for Fig. 2(a) was chosen to be as far removed as possible from the major planes of the crystal in order to give the effect of tilting off [110] into a random plane. Because of the results given above for planar channeling, an attempt was made to associate the peak of the shoulder in Fig. 2(a) with the breakthrough angle for rows. The breakthrough angle for the continuum row potential averaged over thermal vibrations[12] is 0.57° [13]; this does not agree at all well with the position of the shoulder. To explore the possibility that the plane chosen for Fig. 2(a) was not sufficiently random, calculations were done for two other planes with results shown in Figs. 2(b) and 2(c).

The curves of Fig. 2 suggested that it would be of interest to make a contour plot of the nuclear reaction probability for a whole quadrant around the [110] direction.[14] Values of this probability were computed at several hundred points out to 4°–5° from [110]. These calculations were done for the same depth and beam divergence as Fig. 2. Use of a greater depth would have given better correspondence with the experiments but would also have added considerably to the computing time, which was several hours. The results shown in Fig. 1 as well as other calculations of depth dependence indicate that the features of the contour plot would be a bit sharper and more pronounced at somewhat greater depth but very similar to those for the chosen depth. To construct the contours, smooth curves were drawn through groups of calculated points, and the locations of points on the contours determined. After the many points on each contour were plotted, the curve through them was smoothed. The results are shown in Fig. 3. It was difficult to determine the exact form of some

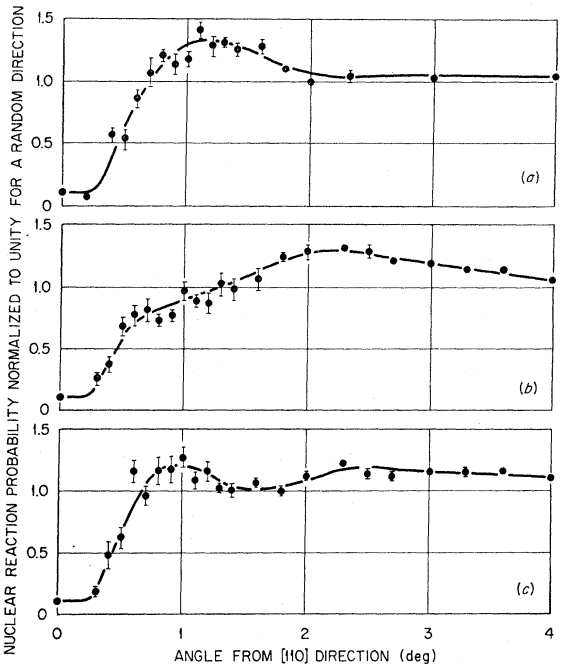


FIG. 2. Nuclear reaction probability for tilts off the [110] direction into various planes. The angles between the tilting planes and the (002) plane are (a) 37.5°, (b) 45°, and (c) 20°.

[12] Expressions for these potentials have been developed by Erginsoy [C. Erginsoy, in *Interaction of Radiation with Solids*, edited by Adli Bishay (Plenum Press, Inc., New York, 1967), pp. 341–60; Bull. Am. Phys. Soc. **12**, 80 (1967)] and by the author (unpublished).

[13] Values for breakthrough angles determined by continuum potentials averaged over thermal vibrations are in very good agreement with values obtained by detailed analysis of groups of trajectories.

[14] A copper *L*-shell x-ray yield contour near [110] for experiments using 70-keV protons has been given by J. M. Khan, D. L. Potter, R. D. Worley, and H. P. Smith, Jr., Phys. Rev. **148**, 413 (1966). Their figure shows less detail than the present contour plot, and they did not draw the conclusions given here. Also, a contour plot of the intensity of protons (incident energy = 120 keV) backscattered from copper has been observed by Rainer Behrisch (to be published).

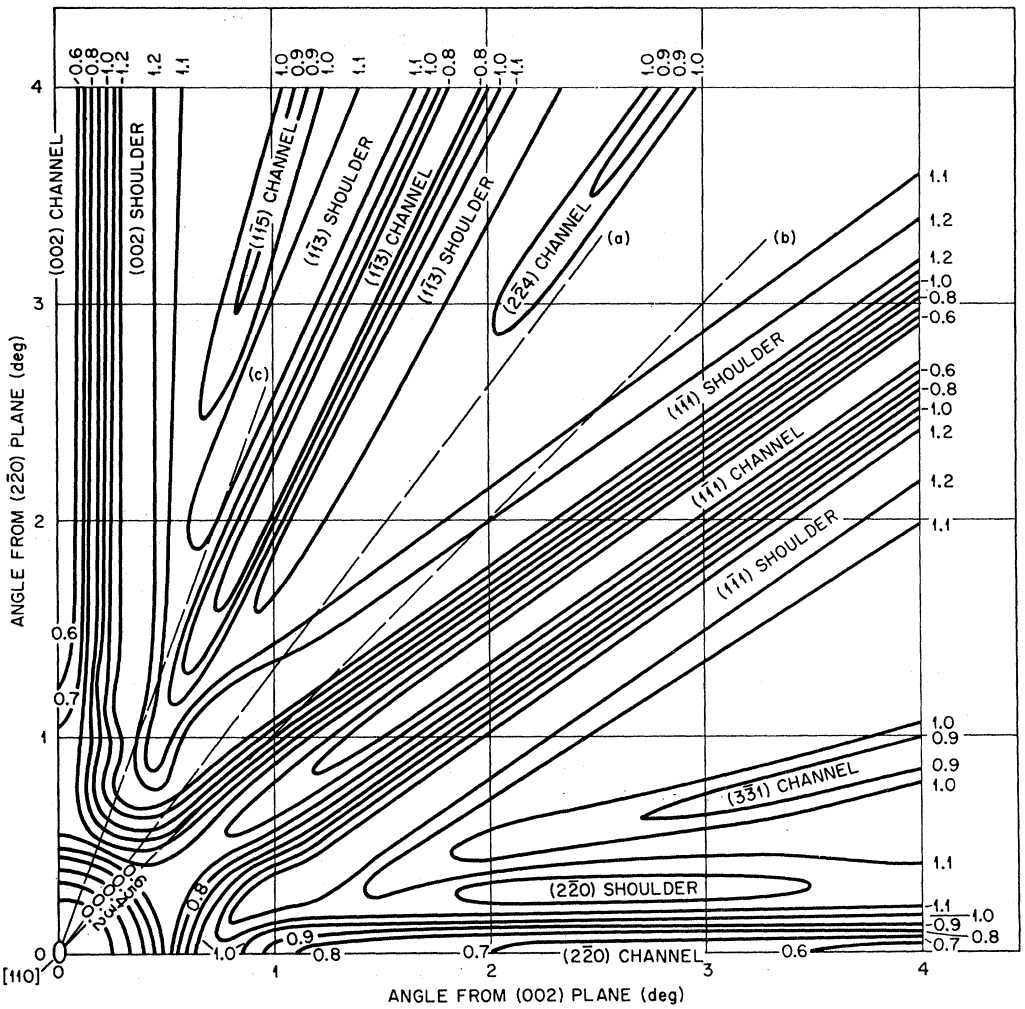


FIG. 3. Contour plot of nuclear reaction probability for directions near the [110] direction. The reaction probability is normalized to unity for a random direction. The dashed lines correspond to the parts of Fig. 2.

contours in the region about 1° from [110]. However, it is felt that these contours are at least as complex as shown. The complexities appear to be due to the intersections of shoulders of various planar channels. As seen in Fig. 3, the maxima of the curves in all three parts of Fig. 2, whether simple or complex, correlate quite well with crossings of shoulders of planar channels.

In order to test the influence of choice of potential on the results, calculations were done at a few selected points using the Bohr potential.[15] The results did not differ strikingly from those using the potential mentioned earlier. Also, a few calculations were done without thermal vibrations. The principal difference from the more extensive calculations with thermal vibrations appeared to be an approximate doubling of channel widths. It is felt that the general nature of the results presented in this paper does not depend on the choice of potential or on the model of thermal vibrations used.

The results of the present calculations indicate that the peak of the shoulder observed in various planar-channeling phenomena can be correlated quite well with the breakthrough angle for planes. However, the breakthrough angle for rows is unrelated to the position of the shoulder of a row channel. This lack of correlation is perhaps not surprising because of the unlikelihood of a direct encounter of a trajectory with a row. The breakthrough angle for rows does appear to determine the rather sharp boundary in Fig. 3 between regions in which row and planar effects predominate.

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